



wwPDB EM Validation Summary Report ⓘ

May 4, 2025 – 09:19 PM EDT

PDB ID : 6C04 / pdb_00006c04
EMDB ID : EMD-7320
Title : Mtb RNAP Holo/RbpA/double fork DNA -closed clamp
Authors : Darst, S.A.; Campbell, E.A.; Boyaci Selcuk, H.; Chen, J.; Lilic, M.
Deposited on : 2017-12-27
Resolution : 3.27 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

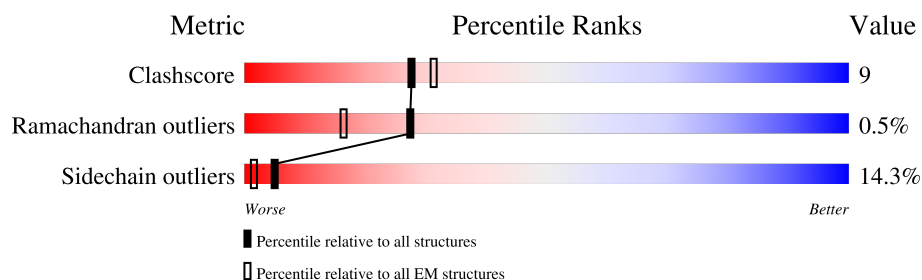
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





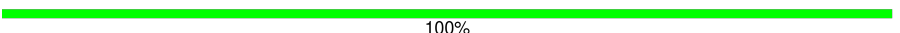
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
2	C	1179	
3	D	1326	
4	E	110	
5	F	531	
6	J	111	
7	H	31	

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Mol	Chain	Length	Quality of chain
7	O	31	 90%10%
8	G	26	 62%8%31%
8	P	26	 100%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 27982 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1724	1085	297	339	3		
1	B	237	Total	C	N	O	S	0	0
			1775	1120	304	348	3		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8585	5378	1507	1661	39		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1179	LEU	-	expression tag	UNP V9Z879
C	1180	ALA	-	expression tag	UNP V9Z879
C	1181	ARG	-	expression tag	UNP V9Z879
C	1182	HIS	-	expression tag	UNP V9Z879
C	1183	GLY	-	expression tag	UNP V9Z879
C	1184	GLY	-	expression tag	UNP V9Z879
C	1185	SER	-	expression tag	UNP V9Z879

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1267	Total	C	N	O	S	0	0
			9881	6190	1795	1854	42		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A0A045J9E2
D	0	ALA	-	expression tag	UNP A0A045J9E2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP A0A045J9E2
D	1318	HIS	-	expression tag	UNP A0A045J9E2
D	1319	HIS	-	expression tag	UNP A0A045J9E2
D	1320	HIS	-	expression tag	UNP A0A045J9E2
D	1321	HIS	-	expression tag	UNP A0A045J9E2
D	1322	HIS	-	expression tag	UNP A0A045J9E2
D	1323	HIS	-	expression tag	UNP A0A045J9E2
D	1324	HIS	-	expression tag	UNP A0A045J9E2

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP A0A0T9N9K3

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	319	Total	C	N	O	S	0	0
			2508	1566	453	480	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP A0A045HD00
F	-1	PRO	-	expression tag	UNP A0A045HD00
F	0	HIS	-	expression tag	UNP A0A045HD00

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	108	Total	C	N	O	S	0	0
			881	543	168	167	3		

- Molecule 7 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	31	Total	C	N	O	P	0	0
			634	305	114	185	30		
7	H	22	Total	C	N	O	P	0	0
			454	218	82	132	22		

- Molecule 8 is a DNA chain called DNA (26-MER).

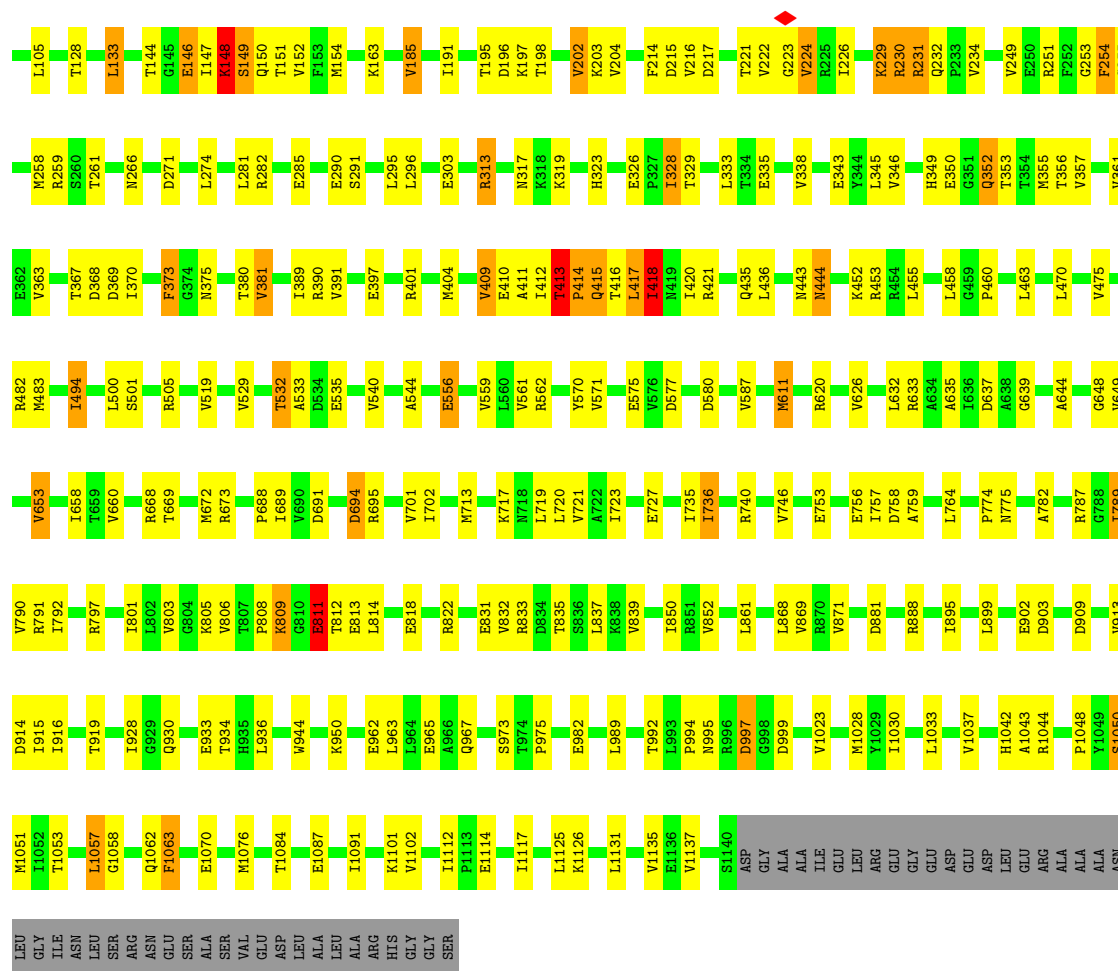
Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	26	Total	C	N	O	P	0	0
			526	254	94	153	25		
8	G	18	Total	C	N	O	P	0	0
			362	176	64	105	17		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	

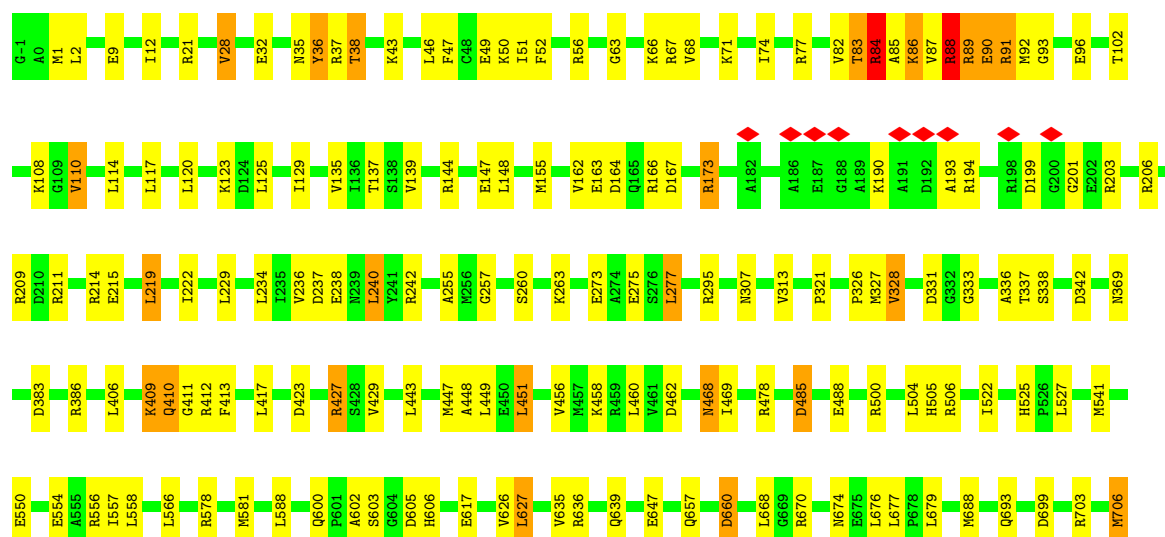
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

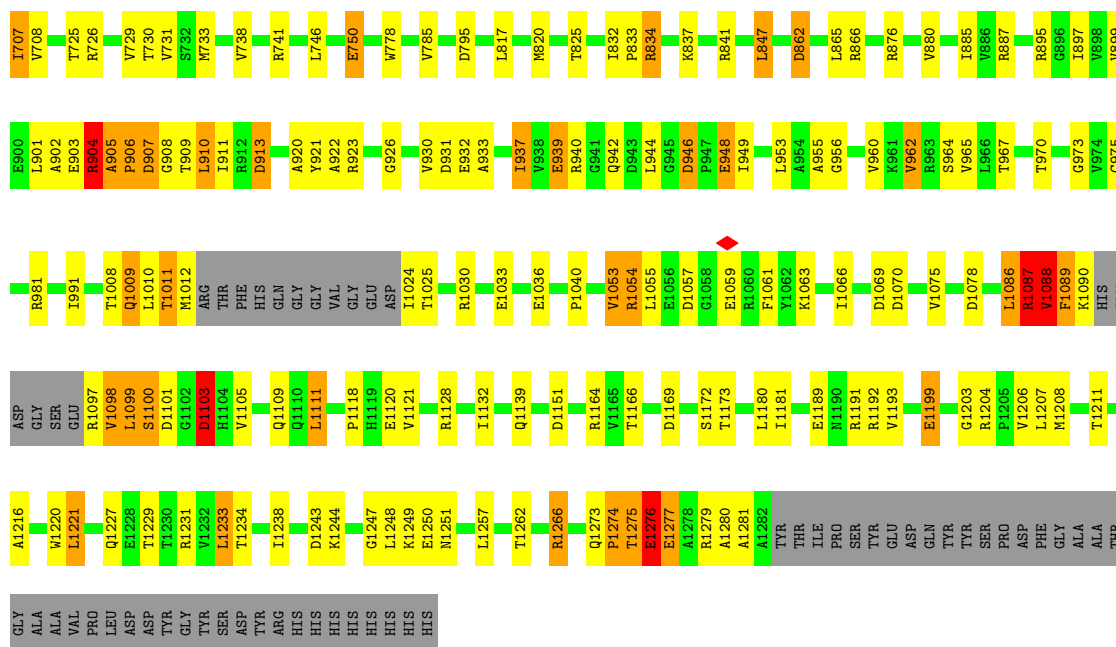
Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	



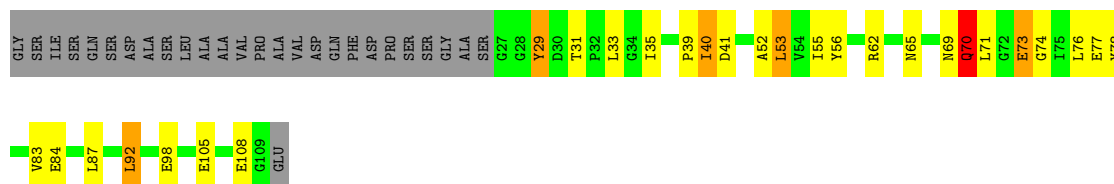
● Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 70% 21%

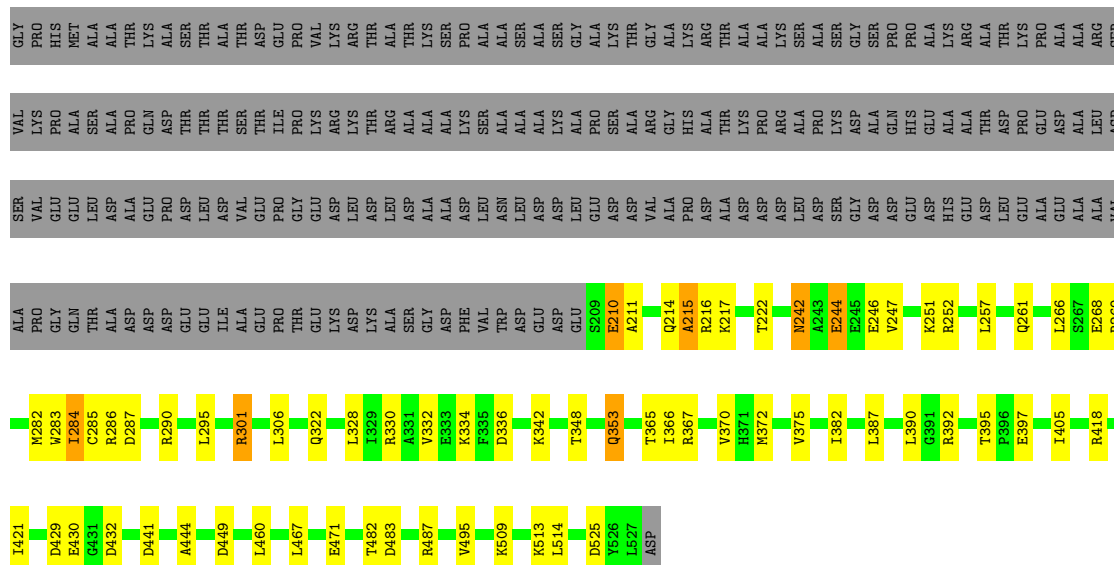




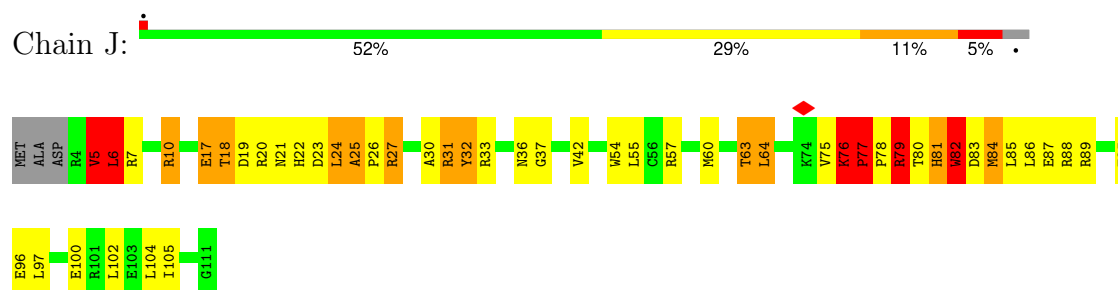
- Molecule 4: DNA-directed RNA polymerase subunit omega



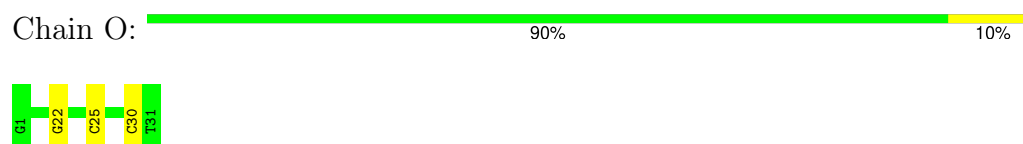
- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 6: RNA polymerase-binding protein RbpA



- Molecule 7: DNA (31-MER)



- Molecule 7: DNA (31-MER)



- Molecule 8: DNA (26-MER)



There are no outlier residues recorded for this chain.

- Molecule 8: DNA (26-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	6.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.539	Depositor
Minimum map value	-1.657	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	0.372	Depositor
Map size (\AA)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	1/1750 (0.1%)	0.53	3/2380 (0.1%)
1	B	0.75	9/1802 (0.5%)	0.63	4/2454 (0.2%)
2	C	0.45	5/8743 (0.1%)	0.63	11/11859 (0.1%)
3	D	0.81	63/10045 (0.6%)	0.69	33/13581 (0.2%)
4	E	0.59	2/662 (0.3%)	0.75	3/901 (0.3%)
5	F	0.31	1/2539 (0.0%)	0.48	0/3426
6	J	1.19	12/897 (1.3%)	2.38	15/1210 (1.2%)
7	H	0.42	1/509 (0.2%)	0.51	0/784
7	O	0.31	0/710	0.52	0/1095
8	G	0.27	0/405	0.50	0/622
8	P	0.31	0/589	0.48	0/906
All	All	0.63	94/28651 (0.3%)	0.75	69/39218 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	3
3	D	0	4
All	All	0	7

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	92	MET	C-O	-13.40	1.07	1.24
3	D	88	ARG	C-O	-13.35	1.06	1.24
3	D	52	PHE	C-O	-12.48	1.07	1.24
1	B	147	VAL	C-O	-12.00	1.09	1.24
3	D	51	ILE	C-O	-10.99	1.11	1.23

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	77	PRO	CA-C-N	48.09	179.95	119.84
6	J	77	PRO	C-N-CA	48.09	179.95	119.84
3	D	1011	THR	N-CA-C	13.46	125.95	111.28
6	J	25	ALA	CA-C-N	12.31	132.28	119.85
6	J	25	ALA	C-N-CA	12.31	132.28	119.85

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	229	LYS	Peptide
2	C	254	PHE	Peptide
2	C	774	PRO	Peptide
3	D	578	ARG	Peptide
3	D	600	GLN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1724	0	1768	28	0
1	B	1775	0	1809	27	0
2	C	8585	0	8508	158	0
3	D	9881	0	9949	221	0
4	E	649	0	645	18	0
5	F	2508	0	2525	46	0
6	J	881	0	861	57	0
7	H	454	0	251	12	0
7	O	634	0	350	5	0
8	G	362	0	206	1	0
8	P	526	0	296	0	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	27982	0	27168	521	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 521 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1089:PHE:CE1	3:D:1109:GLN:NE2	1.91	1.38
6:J:76:LYS:HB2	6:J:77:PRO:CD	1.67	1.23
3:D:1089:PHE:CD1	3:D:1109:GLN:NE2	2.09	1.20
5:F:261:GLN:HG2	6:J:82:TRP:CZ2	1.78	1.17
6:J:76:LYS:HB2	6:J:77:PRO:HD3	1.16	1.15

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/347 (65%)	206 (92%)	18 (8%)	0	100	100
1	B	235/347 (68%)	205 (87%)	30 (13%)	0	100	100
2	C	1109/1179 (94%)	1001 (90%)	106 (10%)	2 (0%)	44	72
3	D	1261/1326 (95%)	1171 (93%)	83 (7%)	7 (1%)	22	52
4	E	81/110 (74%)	71 (88%)	9 (11%)	1 (1%)	11	38
5	F	317/531 (60%)	307 (97%)	9 (3%)	1 (0%)	37	67
6	J	106/111 (96%)	91 (86%)	11 (10%)	4 (4%)	2	16
All	All	3333/3951 (84%)	3052 (92%)	266 (8%)	15 (0%)	27	56

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	904	ARG
3	D	905	ALA
3	D	909	THR

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Mol	Chain	Res	Type
6	J	78	PRO
3	D	1100	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/297 (66%)	165 (85%)	30 (15%)	2	10
1	B	197/297 (66%)	160 (81%)	37 (19%)	1	5
2	C	932/997 (94%)	804 (86%)	128 (14%)	3	14
3	D	1043/1103 (95%)	907 (87%)	136 (13%)	3	15
4	E	69/89 (78%)	55 (80%)	14 (20%)	1	4
5	F	262/429 (61%)	231 (88%)	31 (12%)	4	18
6	J	93/97 (96%)	69 (74%)	24 (26%)	0	1
All	All	2791/3309 (84%)	2391 (86%)	400 (14%)	5	13

5 of 400 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	409	LYS
3	D	962	VAL
6	J	105	ILE
3	D	469	ILE
3	D	706	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	544	HIS
3	D	792	HIS
6	J	28	GLN
3	D	606	HIS
3	D	693	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

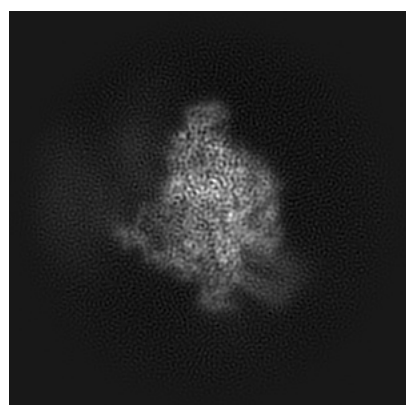
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7320. These allow visual inspection of the internal detail of the map and identification of artifacts.

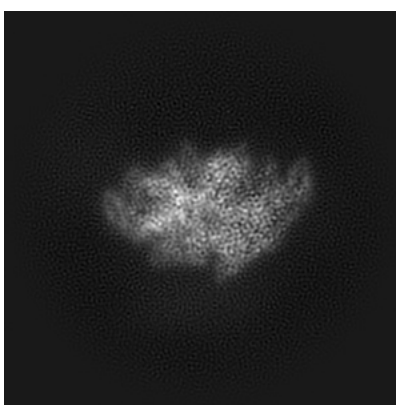
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

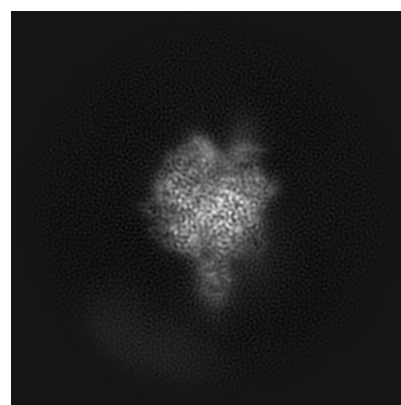
6.1.1 Primary map



X



Y

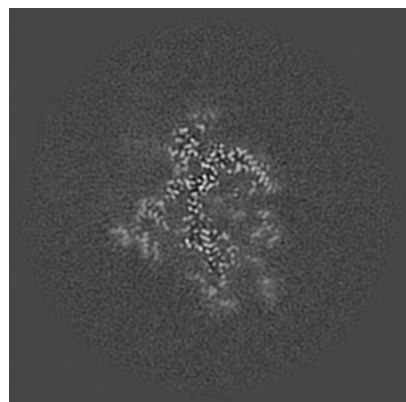


Z

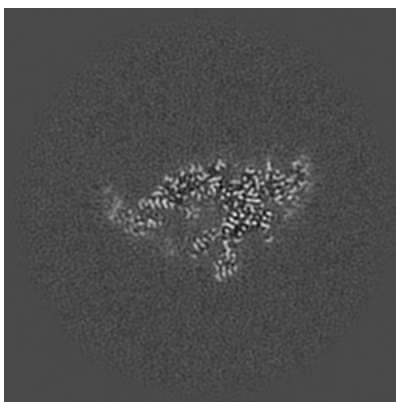
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

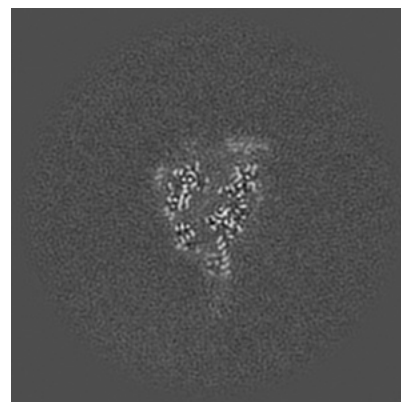
6.2.1 Primary map



X Index: 150



Y Index: 150

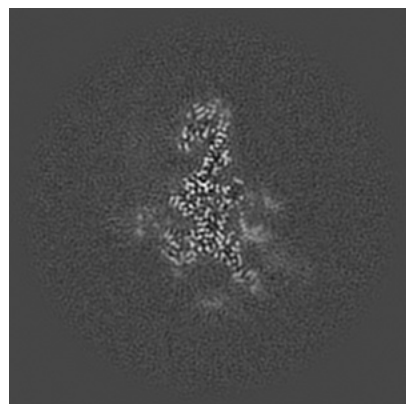


Z Index: 150

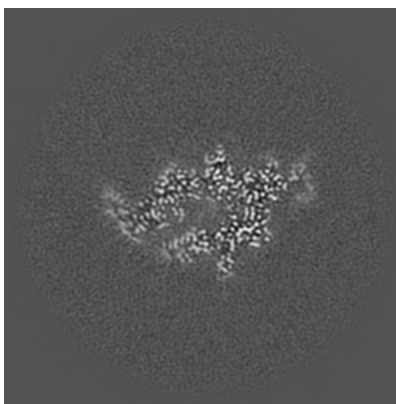
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

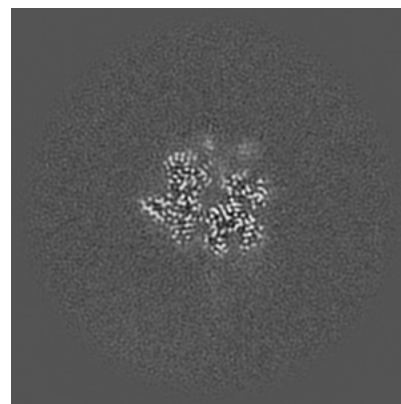
6.3.1 Primary map



X Index: 164



Y Index: 156

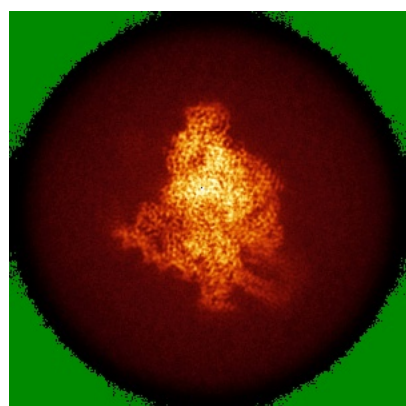


Z Index: 164

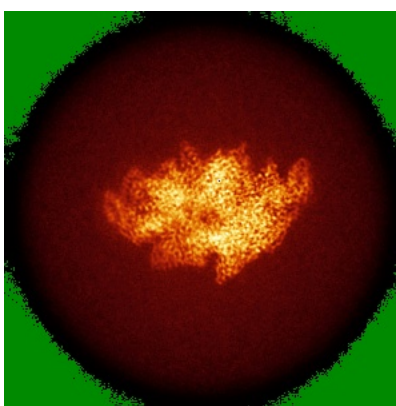
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

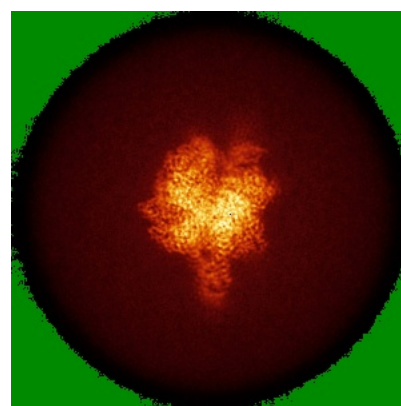
6.4.1 Primary map



X



Y

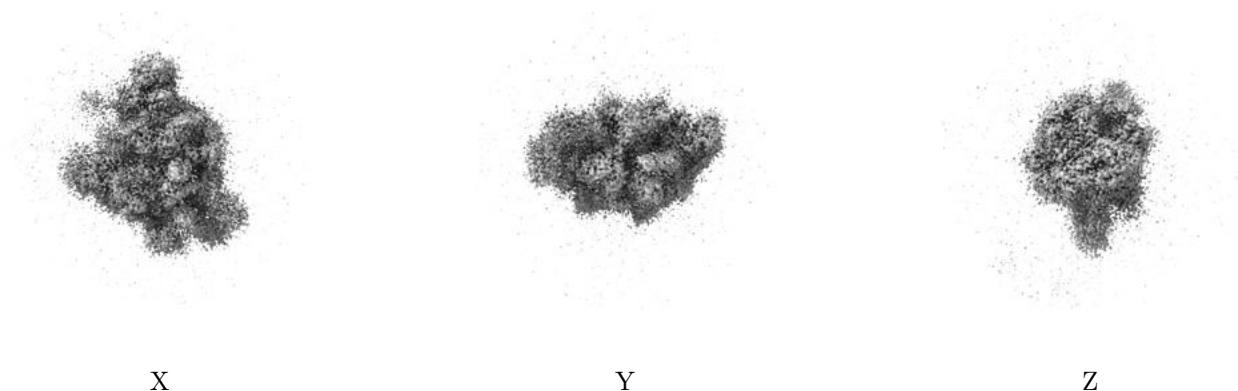


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.372. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

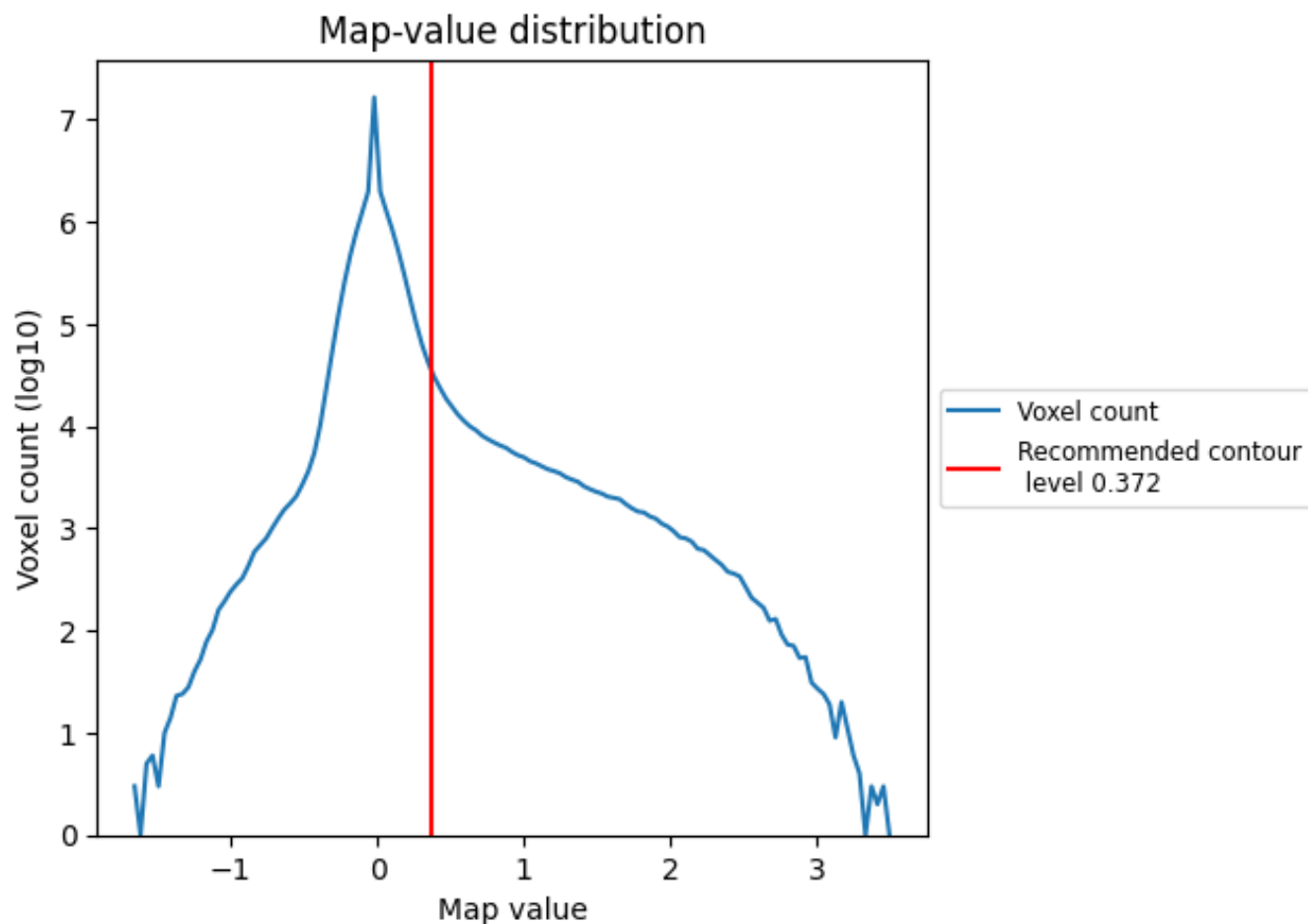
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

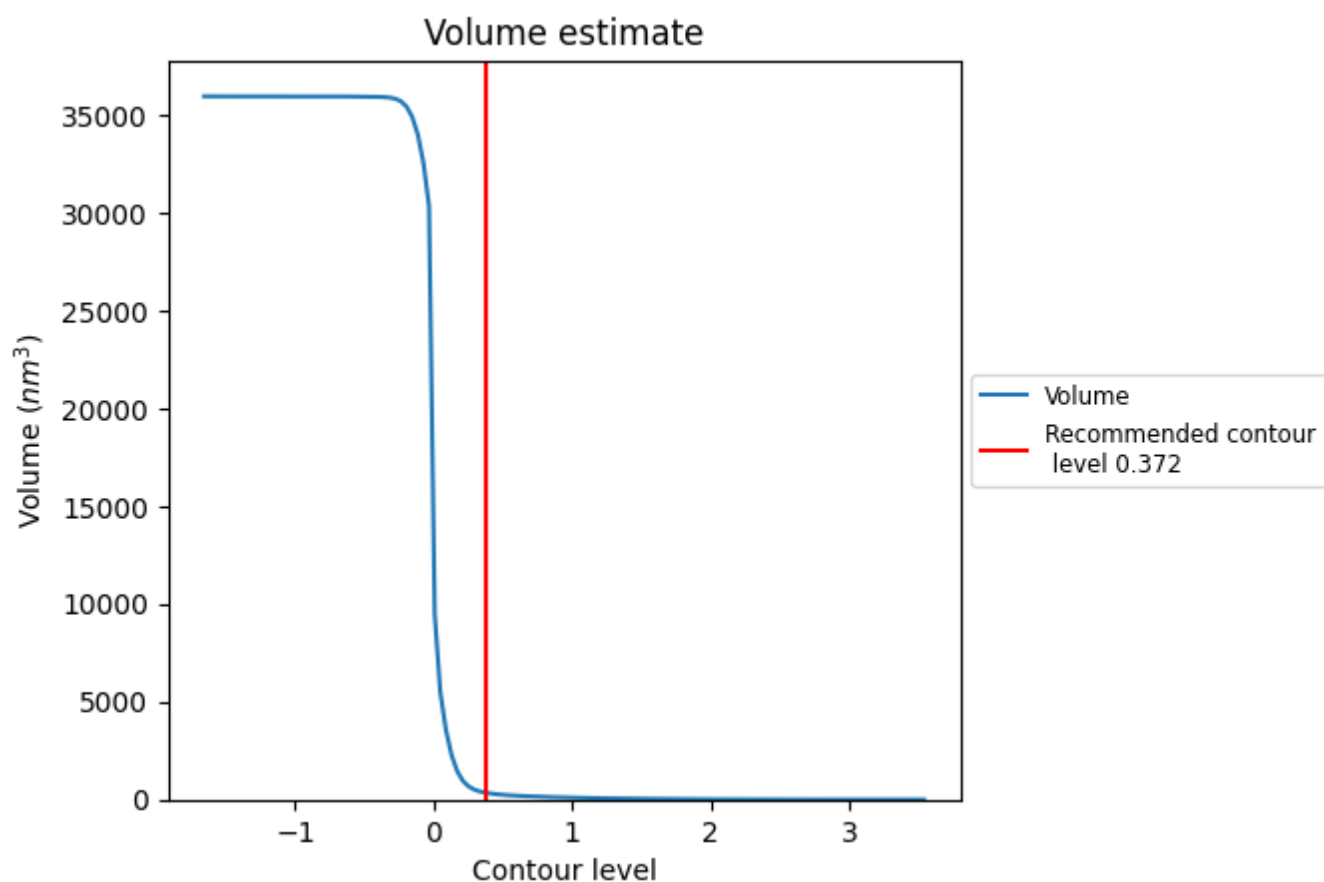
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

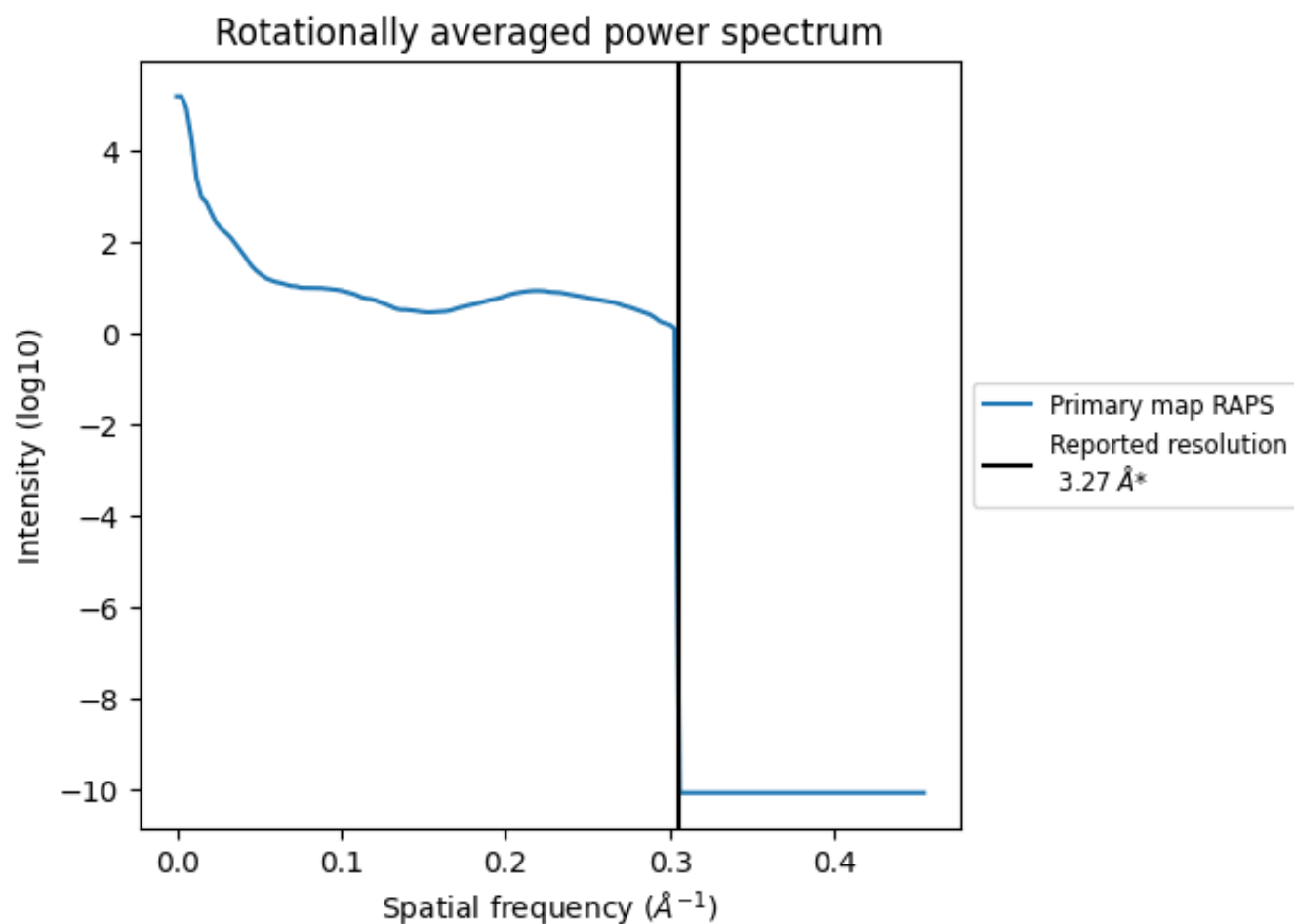
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 354 nm^3 ; this corresponds to an approximate mass of 319 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.306 Å⁻¹

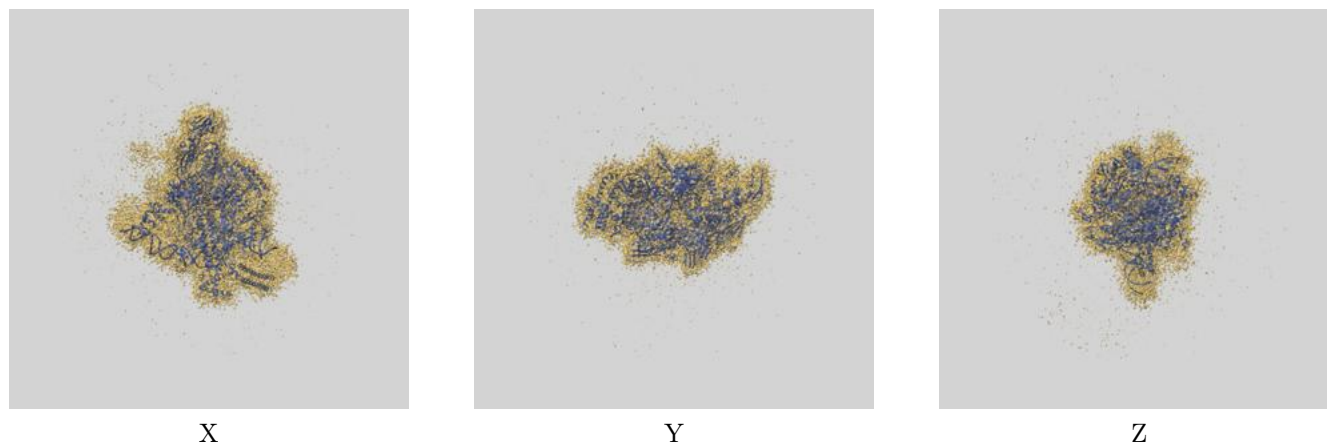
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

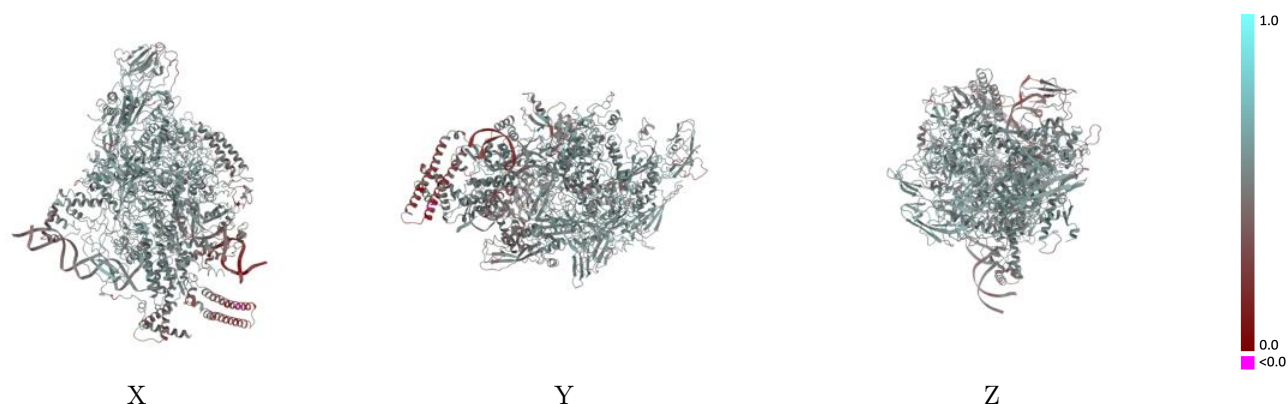
This section contains information regarding the fit between EMDB map EMD-7320 and PDB model 6C04. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.372 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



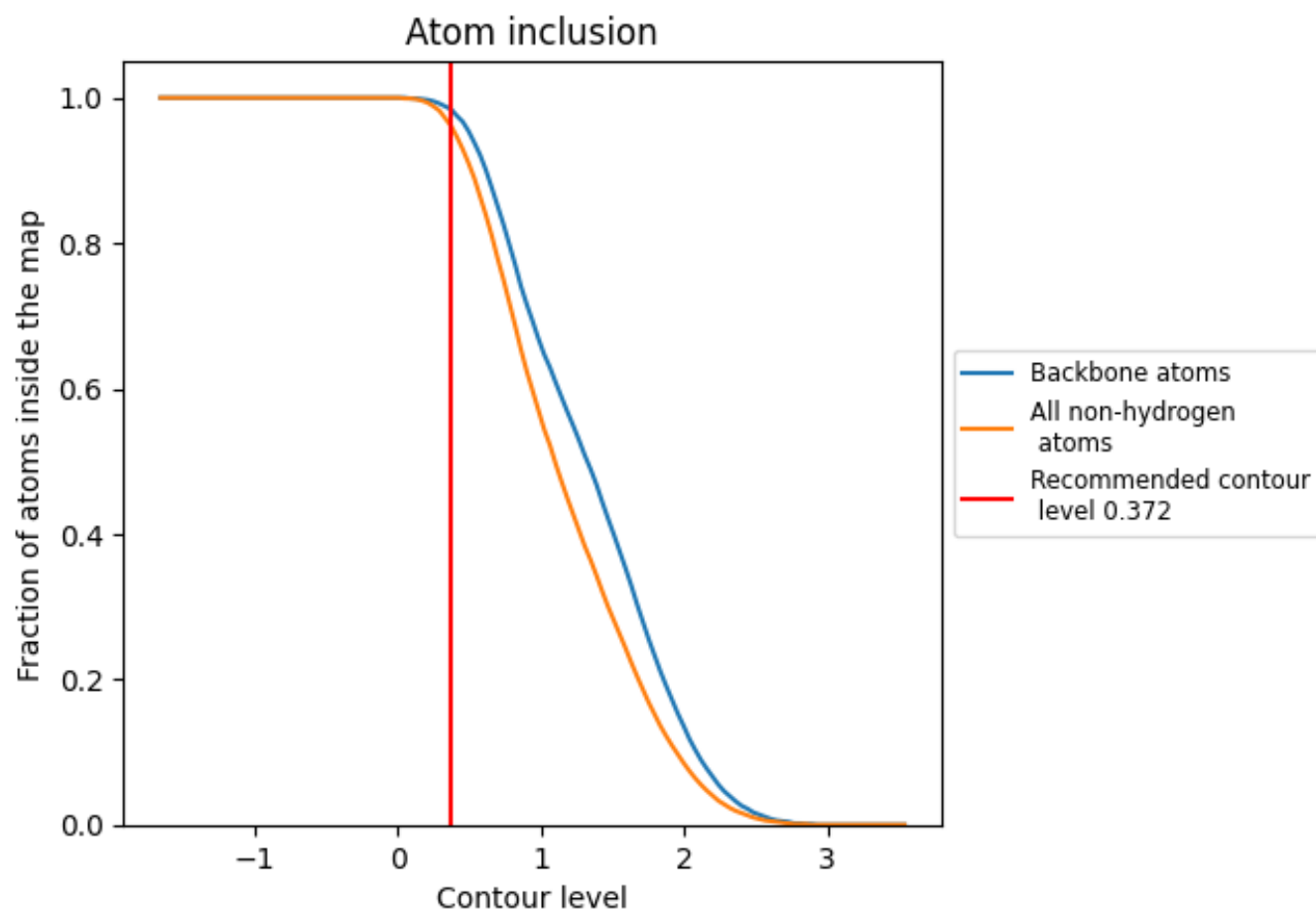
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.372).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.372) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9610	<div></div> 0.5150
A	<div></div> 0.9700	<div></div> 0.5410
B	<div></div> 0.9510	<div></div> 0.5090
C	<div></div> 0.9660	<div></div> 0.5300
D	<div></div> 0.9560	<div></div> 0.5220
E	<div></div> 0.9640	<div></div> 0.5370
F	<div></div> 0.9580	<div></div> 0.4940
G	<div></div> 0.9420	<div></div> 0.3330
H	<div></div> 0.9540	<div></div> 0.3970
J	<div></div> 0.9420	<div></div> 0.5010
O	<div></div> 0.9950	<div></div> 0.4560
P	<div></div> 0.9870	<div></div> 0.4520

1.0

0.0

<0.0